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MEMORANDUM FOR PRS (In-House / Contractor Publication)

FROM: PROI (STINFO)

18 June 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-AB-2002-146
Karl Christe (ERC) et al., "Synthesis and Structural Characterization of Nitrogen Containing High
Energy Density Materials" (abstract only)

Int'l Congress, Int'l Union of Crystallography (Geneva, 6-15 August 2002) (<u>Deadline = 14 July 2002</u>)

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Synthesis and Structural Characterization of Nitrogen Containing High Energy Density Materials

Ashwani Vij, Karl O. Christe, Vandana Vij, William W. Wilson, Fook S. Tham, Ralf Haiges, Michael Gerken and Xiongzhi Zhang

Propulsion Directorate and Advanced Concepts Division, Air Force Research Laboratory, Edwards Air Force Base, CA 93524, Loker Hydrocarbon Research Institute and Department of Chemistry, University of Southern California, Los Angeles, CA 90089 and Department of Chemistry, University of California, Riverside, CA 92521

Polynitrogen compounds are of great interest as High Energy Density Materials (HEDM). Single crystal x-ray crystallography plays a crucial role in the characterization of these materials and their precursors. In this paper, we report the crystal structures of the novel N_5^+ cation in N_5^+ Sb₂F₁₁, which is the first stable polynitrogen species to be discovered in a century since the discovery of the azide ion. The other HEDM materials synthesized and characterized are N_2F^+ $M_xF_{2x+1}^-$ (M = As or Sb), NOF_2^+ AsF₆, NF_4^+ Sb₂F₁₁, NF_3F^+ SO₃CF₃, $M(N_3)_3$ (M = As or Sb) and SbCl_x(N_3)_{6-x} (x = 2 or 4). In the case of oxofluorides, oxygen fluorine disorder is frequently encountered and a new method for obtaining valuable structural information from disordered structures is briefly discussed for the NOF_2^+ cation. The techniques employed for handling these energetic materials for x-ray diffraction studies will also be described.

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